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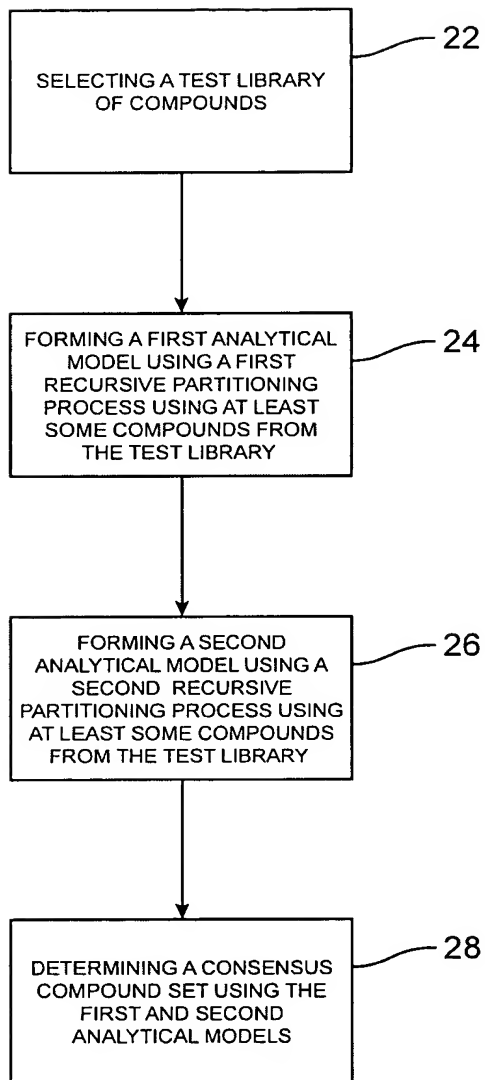


FIG. 1

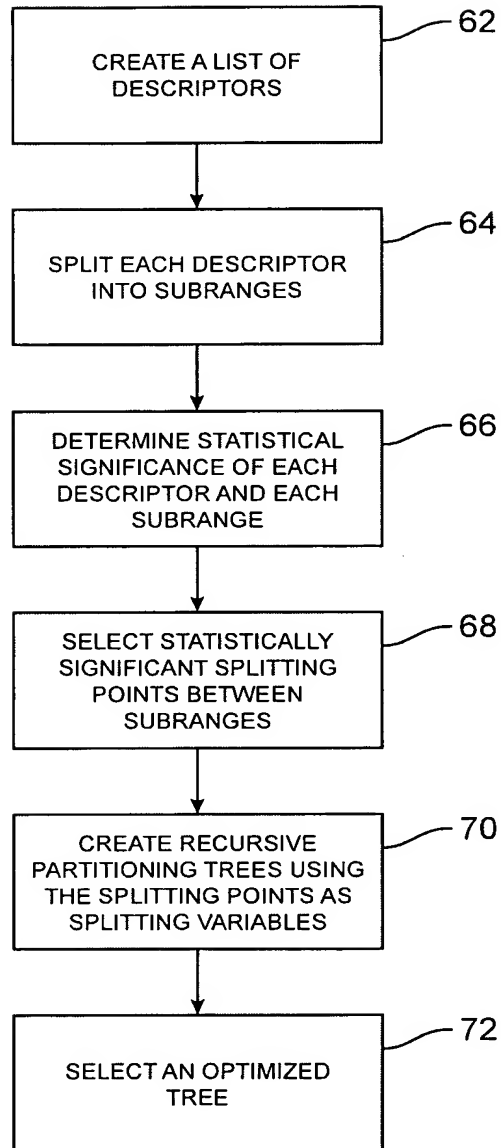


FIG. 2


$$+$$

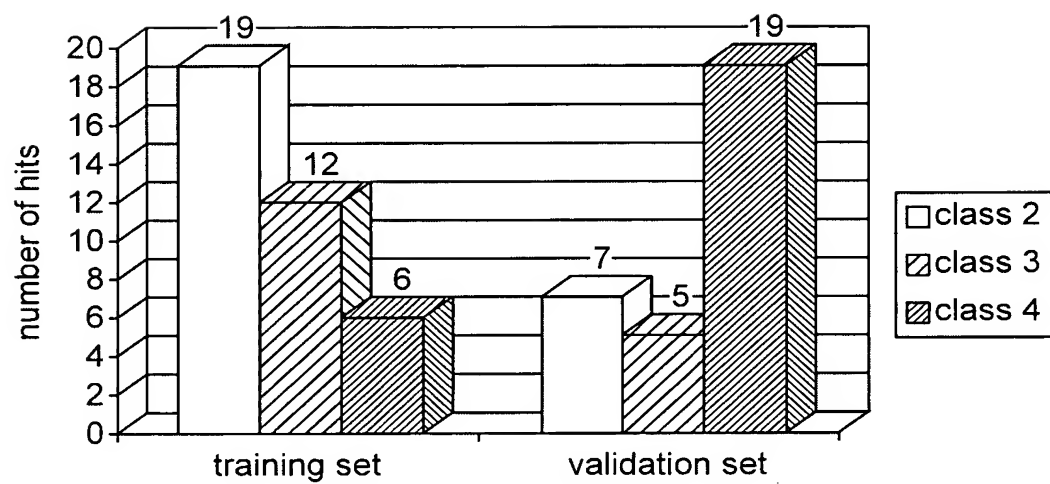


FIG. 4(a)

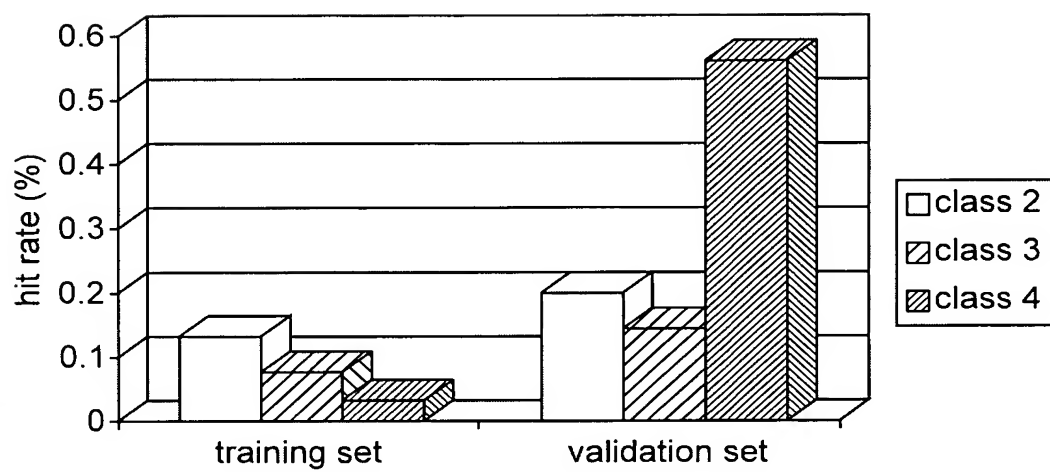


FIG. 4(b)

TABLE I

TD	max. knots	min. samples	% class correct	fold enrichment	% false positives	# selected	# active nodes	# terminal nodes	selected/node
9	85	144	89	14.6	98.2	882	5	27	176.4
9	103	90	100	21.0	97.4	688	7	35	98.3
9	103	54	89	22.8	97.2	562	7	37	80.3
12	107	18	94	65.8	91.8	207	9	59	23.0
12	107	3	94	184.2	77.0	74	11	95	6.7
12	137	1	100	370.0	53.9	39	13	117	3.0

FIG. 5

TABLE II

Training Set												
model	descriptor	TD	max. knots	min. samples	% class correct	fold enrichment	cpds	total	consensus	% class correct	fold enrichment	% false positives
consensus model 1	C45	9	85	144	89	14.6	882	1245	451	78	24.8	96.9
	C45	9	90	144	83	14.8	814					
consensus model 2	C45	9	85	144	89	14.6	882	1199	632	83	19.0	97.6
	C45	9	80	144	89	13.5	949					
consensus model 3	C45	9	80	144	89	13.5	949	1493	411	73	25.3	96.8
	C45	9	85	144	89	14.6	882					
	C45	9	90	144	83	14.8	814					
consensus model 4	C45	9	85	144	89	14.6	882	996	91	83	114.3	84.6
	C45	12	107	18	94	65.8	207					
consensus model 5	C45	12	107	18	94	65.8	207	241	173	94	78.6	90.2
	C45	12	109	18	94	65.8	207					
consensus model 6	C45	12	107	18	94	65.8	207	354	77	94	176.6	77.9
	C45	12	127	18	100	64.4	224					
consensus model 7	C45	9	85	144	89	14.6	882	1563	165	83	63.0	90.9
	BCUT	8	101	144	94	15.8	848					

FIG. 6

TABLE III

							HTS Eligible		
model	descriptor	TD	max. knots	min. samples	% class correct	fold enrichment	cpds	total	consensus
consensus model 1	C45	9	85	144	89	14.6	73106	155699	26354
	C45	9	90	144	83	14.8	68942		
consensus model 2	C45	9	85	144	89	14.6	73106	168263	50449
	C45	9	80	144	89	13.5	105601		
consensus model 3	C45	9	80	144	89	13.5	105601	235436	21821
	C45	9	85	144	89	14.6	73106		
	C45	9	90	144	83	14.8	68942		
consensus model 4	C45	9	85	144	89	14.6	73106	94930	6241
	C45	12	107	18	94	65.8	28065		
consensus model 5	C45	12	107	18	94	65.8	28065	46842	19720
	C45	12	109	18	94	65.8	25632		
consensus model 6	C45	12	107	18	94	65.8	28065	60999	9987
	C45	12	127	18	100	64.4	30056		
consensus model 7	C45	9	85	144	89	14.6	73106	127864	6309
	BCUT	8	101	144	94	15.8	61067		

FIG. 7

TABLE IV

							Validation Set							
model	descriptor	TD	max. knots	min. samples	% class correct	fold enrichment	cpds	total	consensus	class 4 hits	class 3 hits	class 2 hits	fold enrichment (class 4)	fold enrichment (class 4 & 3)
consensus model 1	C45	9	85	144	89	14.6	2242	2323	1351	18	4	5	31.7	13.0
	C45	9	90	144	83	14.8	1432							
consensus model 2	C45	9	85	144	89	14.6	2242	2342	1553	18	5	5	27.6	11.8
	C45	9	80	144	89	13.5	1653							
consensus model 3	C45	9	80	144	89	13.5	1653	2395	1270	18	4	5	33.7	13.9
	C45	9	85	144	89	14.6	2242							
	C45	9	90	144	83	14.8	1432							
consensus model 4	C45	9	85	144	89	14.6	2242	2267	238	3	3	1	30.0	20.2
	C45	12	107	18	94	65.8	263							
consensus model 5	C45	12	107	18	94	65.8	263	314	210	2	3	1	22.7	19.0
	C45	12	109	18	94	65.8	261							
consensus model 6	C45	12	107	18	94	65.8	263	474	92	2	1	1	51.8	26.1
	C45	12	127	18	100	64.4	303							
consensus model 7	C45	9	85	144	89	14.6	2242	2365	421	9	4	4	50.9	24.7
	BCUT	8	101	144	94	15.8	544							

FIG. 8